Maximum Likelihood Estimation
&
Maximum A Posteriori Probability Estimation

Announcements

1. HW2 (Perceptron, PCA, K-means) will be out today

Recap on Perceptron

Binary classifier: $\text{sign}(w^\top x)$

The Perceptron Alg:

Initialize $w_0 = 0$

For $t = 0 \to \infty$

- feature x_t shows up
- We make a prediction $\hat{y}_t = \text{sign}(w_t^\top x_t)$
- Check if $\hat{y}_t$ equal to y_t
- We update $w_{t+1} = w_t + \mathbf{1}(\hat{y}_t \neq y_t) y_t x_t$

Q: how to apply this on a static dataset $\mathscr{D} = \{x_i, y_i\}_{i=1}^n$?

Q: If data has margin $y_i(x_i^\top w^\star) \geq \gamma$, does it guarantee to converge to $w^\star$?

Objective for today:

Understand the two common statistical learning framework: MLE and MAP

Outline for today:

1. Maximum Likelihood estimation (MLE)

2. Maximum a posteriori probability (MAP)

Ex 1: Estimating the probability of a coin flip

We toss a coin n times (independently), we observe the following outcomes:

$\mathscr{D} = \{y_i\}_{i=1}^n, y_i \in \{-1,1\}$ ($y_i = 1$ means head in i's trial, -1 means tail)

Q: assume $y_i \sim$ Bernoulli($\theta^\star$), how to estimate $\theta^\star$ given $\mathscr{D}$?

$$\hat{\theta} = \frac{\sum_{i=1}^n \mathbf{1}(y_i = 1)}{n}$$

Let's make this rigorous!

Maximum Likelihood Estimation

We toss a coin n times (independently), we observe the following outcomes:

$\mathscr{D} = \{y_i\}_{i=1}^n, y_i \in \{-1,1\}$ ($y_i = 1$ means head in i's trial, -1 means tail)

If the probability of getting head is $\theta \in [0,1]$, what is the probability of observing the data $\mathscr{D}$ (i.e., likelihood)?

$$P(\mathscr{D} \mid \theta) = \theta^{n_1}(1-\theta)^{n-n_1}$$

MLE Principle: Find θ that **maximizes the likelihood** of the data:

$$\hat{\theta}_{mle} = \arg \max_{\theta \in [0,1]} P(\mathscr{D} \mid \theta)$$

Maximum Likelihood Estimation

We toss a coin n times (independently), we observe the following outcomes:

$$\mathscr{D} = \{y_i\}_{i=1}^{n}, y_i \in \{-1,1\}$$ ($y_i = 1$ means head in i's trial, -1 means tail)

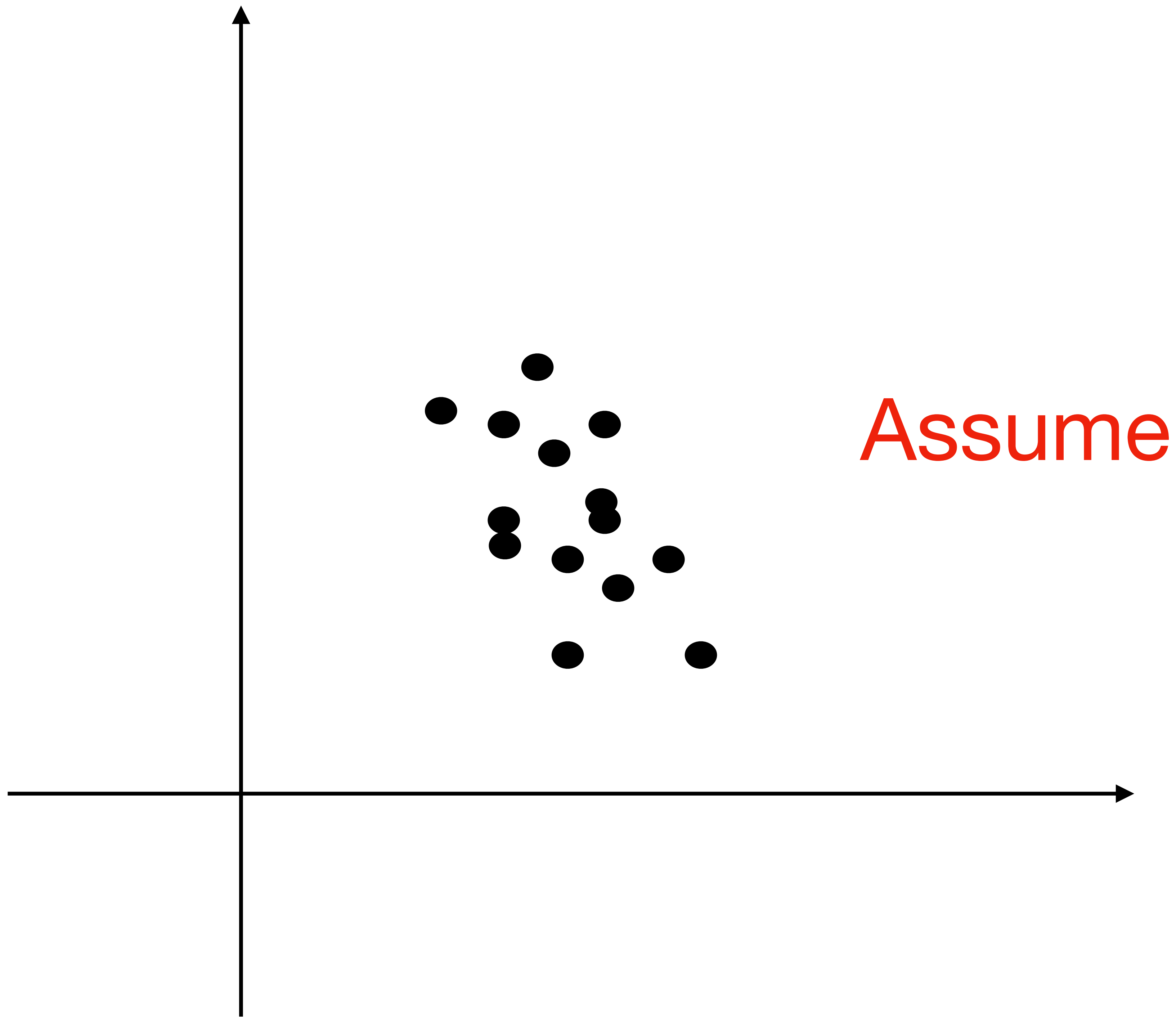
MLE Principle: Find θ that maximizes the likelihood of the data:

$$\hat{\theta}_{mle} = \arg\max_{\theta \in [0,1]} P(\mathscr{D} \mid \theta) = \arg\max_{\theta \in [0,1]} \theta^{n_1}(1-\theta)^{n-n_1}$$

$$= \arg\max_{\theta \in [0,1]} \ln(\theta^{n_1}(1-\theta)^{n-n_1})$$

$$= \arg\max_{\theta \in [0,1]} n_1 \ln(\theta) + (n-n_1)\ln(1-\theta) = \frac{n_1}{n}$$

Ex 2: Estimate the mean



$$\mathscr{D} = \{x_i\}_{i=1}^n, x_i \in \mathbb{R}^d$$

Assume data is from $\mathcal{N}(\mu^\star, I)$, want to estimate $\mu^\star$ from the data $\mathscr{D}$

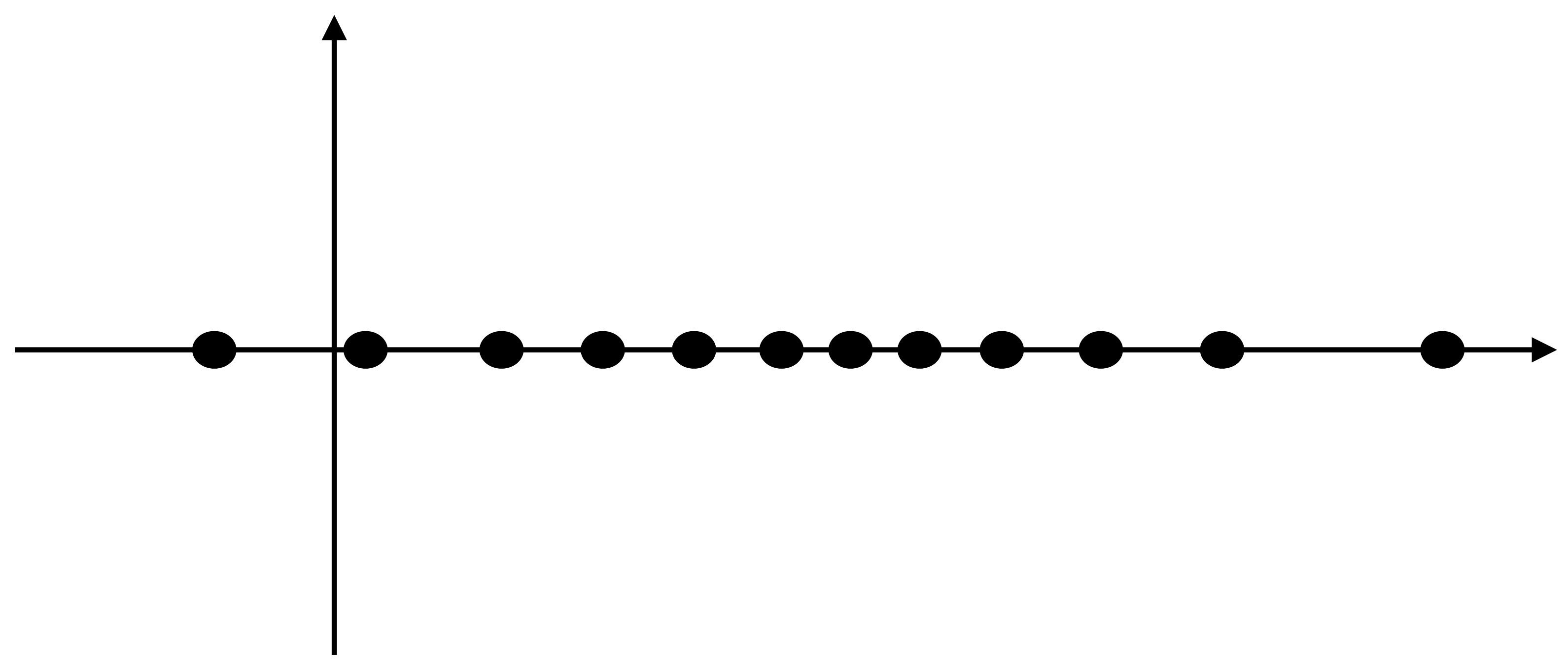
Let's apply the MLE Principle:

Step 1: $P(\mathscr{D} \mid \mu) = \prod_{i=1}^n \frac{1}{\sqrt{(2\pi)^d}} \exp\left(-\frac{1}{2}(x_i - \mu)^\top (x_i - \mu) \right)$

Step 2: apply log and maximize the log-likelihood:

$$\arg\max_\mu \sum_{i=1}^n -(x_i - \mu)^\top (x_i - \mu) \Rightarrow \hat{\mu}_{mle} = \sum_{i=1}^n x_i / n$$

Q: Estimate the mean and variance



$$\mathscr{D} = \{x_i\}_{i=1}^n, x_i \in \mathbb{R}$$

Assume data is from $\mathcal{N}(\mu^\star, \sigma^2)$, want to estimate $\mu^\star, \sigma$ from the data $\mathscr{D}$

Let's apply the MLE Principle:

Step 1: $P(\mathscr{D} \mid \mu, \sigma) = \prod_{i=1}^n \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}(x_i - \mu)^2/\sigma^2\right)$

Step 2: apply log and maximize the log-likelihood:

$$\arg\max_{\mu,\sigma>0} \sum_{i=1}^n \left(-(x_i - \mu)^2/\sigma^2 - \ln(\sigma)\right) = ??$$

Some properties of MLE

1. MLE is consistent: if our model assumption is correct (e.g., coin flip follows some Bernoulli distribution), then $\hat{\theta}_{mle} \to \theta^\star,$ as $n \to \infty$

2. When our model assumption is wrong (e.g., we use Gaussian to model data which is from some more complicated distribution), then MLE loses such guarantee

Outline for today:

1. Maximum Likelihood estimation (MLE)

2. Maximum a Posteriori Probability (MAP)

Ex: Estimating the probability of a coin flip

We toss a coin n times (independently), we observe the following outcomes:

$$\mathscr{D} = \{y_i\}_{i=1}^n, y_i \in \{-1,1\}$$ ($y_i = 1$ means head in i's trial, -1 means tail)

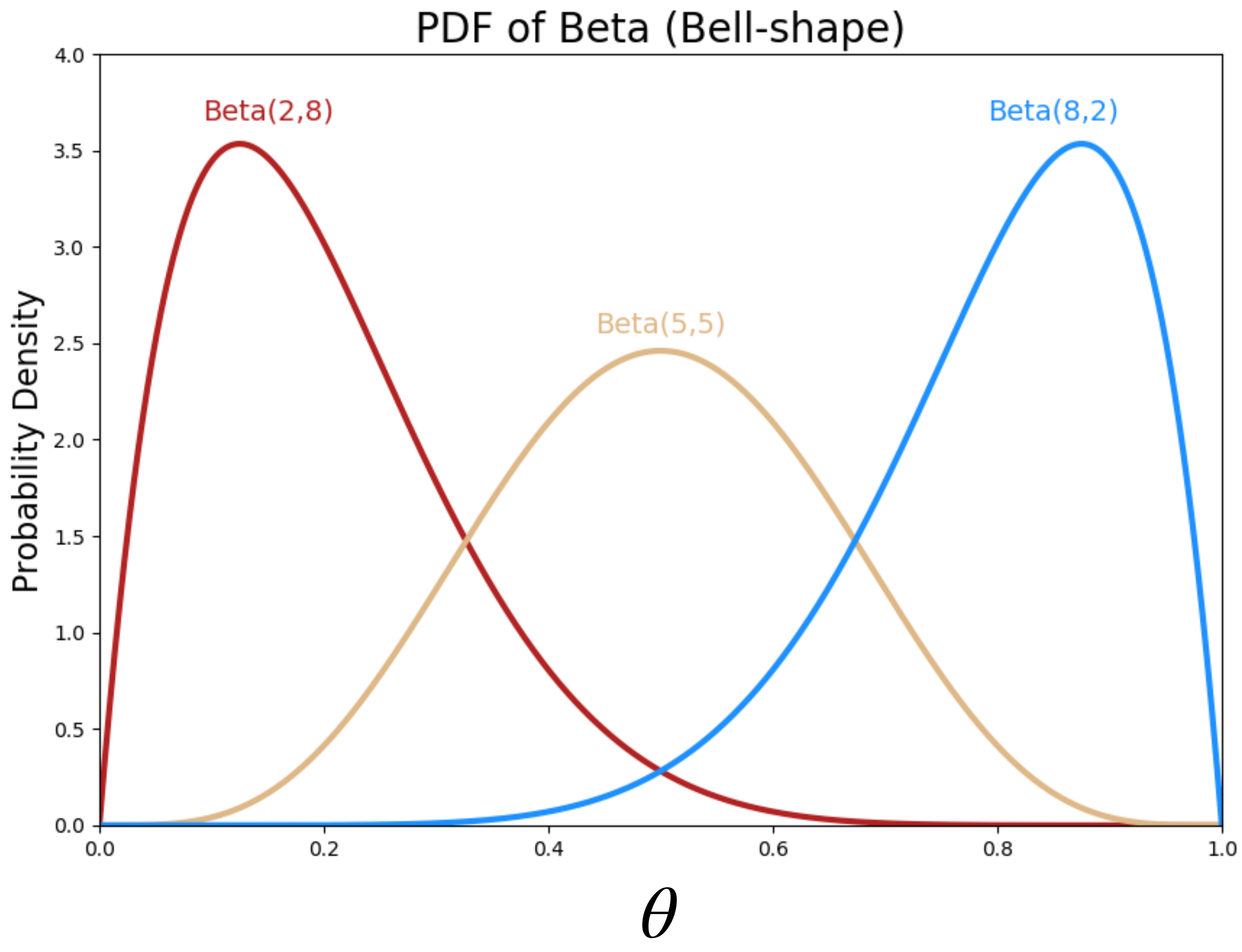
A Bayesian Statistician will treat the optimal parameter $\theta^\star$ being a random variable:

$$\theta^\star \sim P(\theta)$$

Example: $P(\theta)$ being a Beta distribution:

$$P(\theta) = \theta^{\alpha-1}(1-\theta)^{\beta-1}/Z,$$

where $Z = \int_{\theta\in[0,1]} \theta^{\alpha-1}(1-\theta)^{\beta-1} d_\theta$



The Posterior distribution over θ

Now, we have a prior $P(\theta)$, and we have a dataset $\mathscr{D} = \{y_i\}_{i=1}^n$, define posterior distribution:

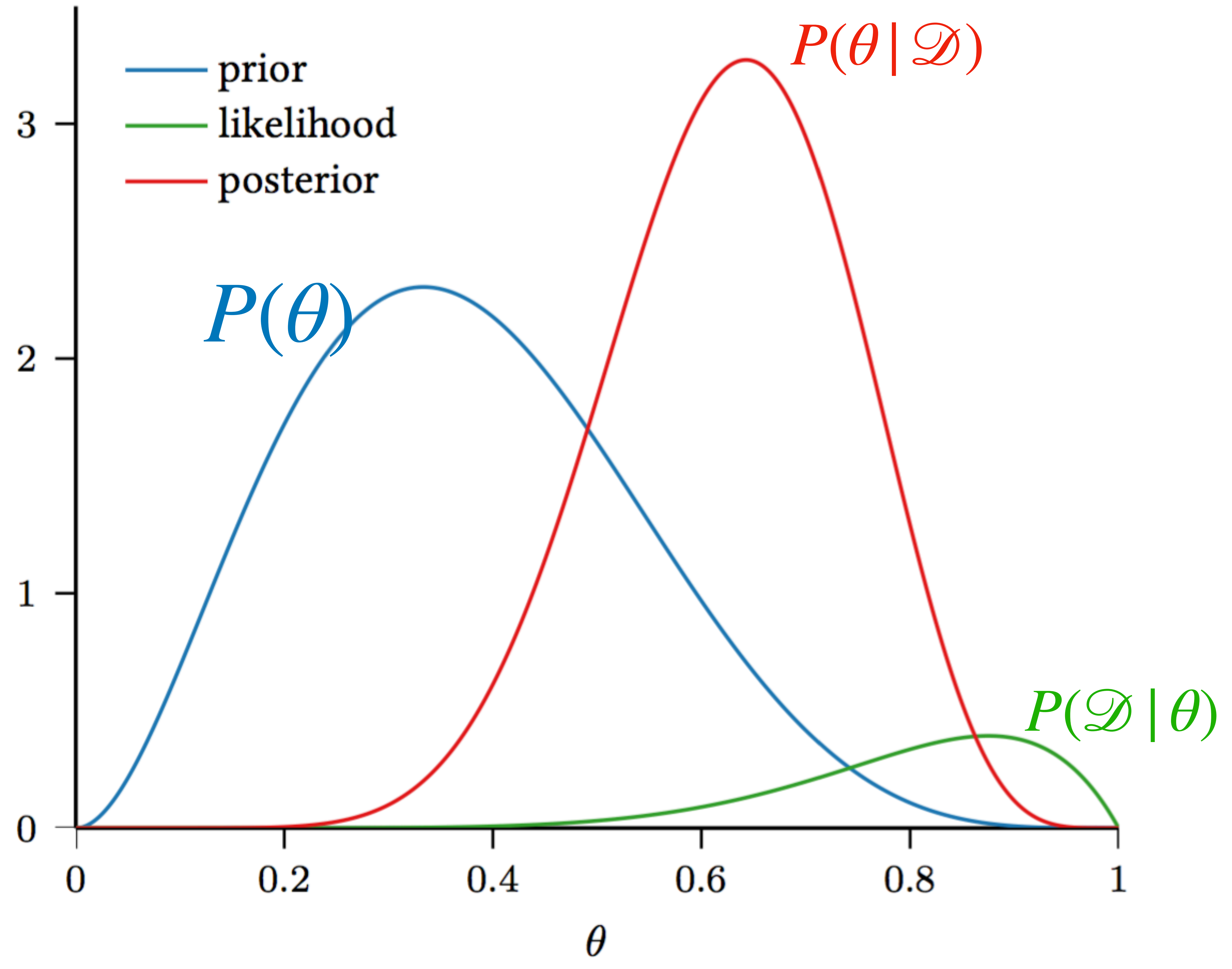
$$P(\theta \mid \mathscr{D})$$

Using Bayes rule, we get:

$$P(\theta \mid \mathscr{D}) = P(\theta)P(\mathscr{D} \mid \theta)/P(\mathscr{D})$$

$$\propto P(\theta)P(\mathscr{D} \mid \theta)$$

Posterior $\propto$ Prior $\times$ Likelihood

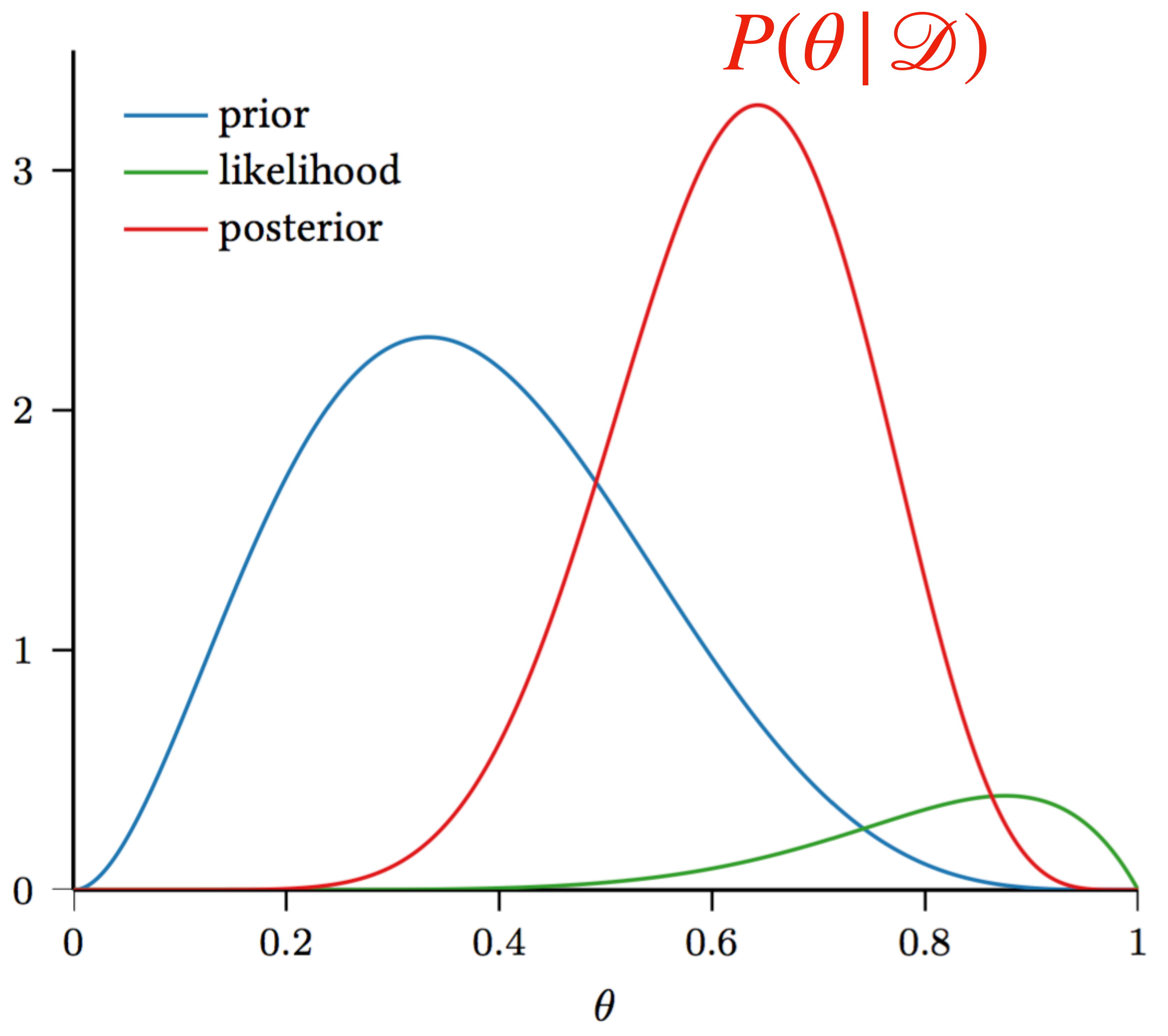


Maximum A Posteriori Probability estimation (MAP)

$$P(\theta \mid \mathscr{D}) \propto P(\theta)P(\mathscr{D} \mid \theta)$$

$$\hat{\theta}_{map} = \arg \max_{\theta \in [0,1]} P(\theta \mid \mathscr{D}) = \arg \max_{\theta \in [0,1]} P(\theta)P(\mathscr{D} \mid \theta)$$

$$= \arg \max_{\theta \in [0,1]} \ln P(\theta) + \ln P(\mathscr{D} \mid \theta)$$



MAP for coin flip

$$\hat{\theta}_{map} = \arg\max_{\theta \in [0,1]} \ln(P(\theta)P(\mathscr{D} \mid \theta))$$

Step 1: specify Prior $P(\theta) \propto \theta^{\alpha-1}(1-\theta)^{\beta-1}$

Step 2: data likelihood $P(\mathscr{D} \mid \theta) = \theta^{n_1}(1-\theta)^{n-n_1}$

Step 3: Compute posterior $P(\theta \mid \mathscr{D}) \propto \theta^{n_1+\alpha-1}(1-\theta)^{n-n_1+\beta-1}$

Step 4: Compute MAP $\hat{\theta}_{map} = \dfrac{n_1 + \alpha - 1}{n + \alpha + \beta - 2}$

$(\alpha - 1, \beta - 1)$ can be understood as some fictions flips: we had $\alpha - 1$ hallucinated heads, and $\beta - 1$ hallucinated tails

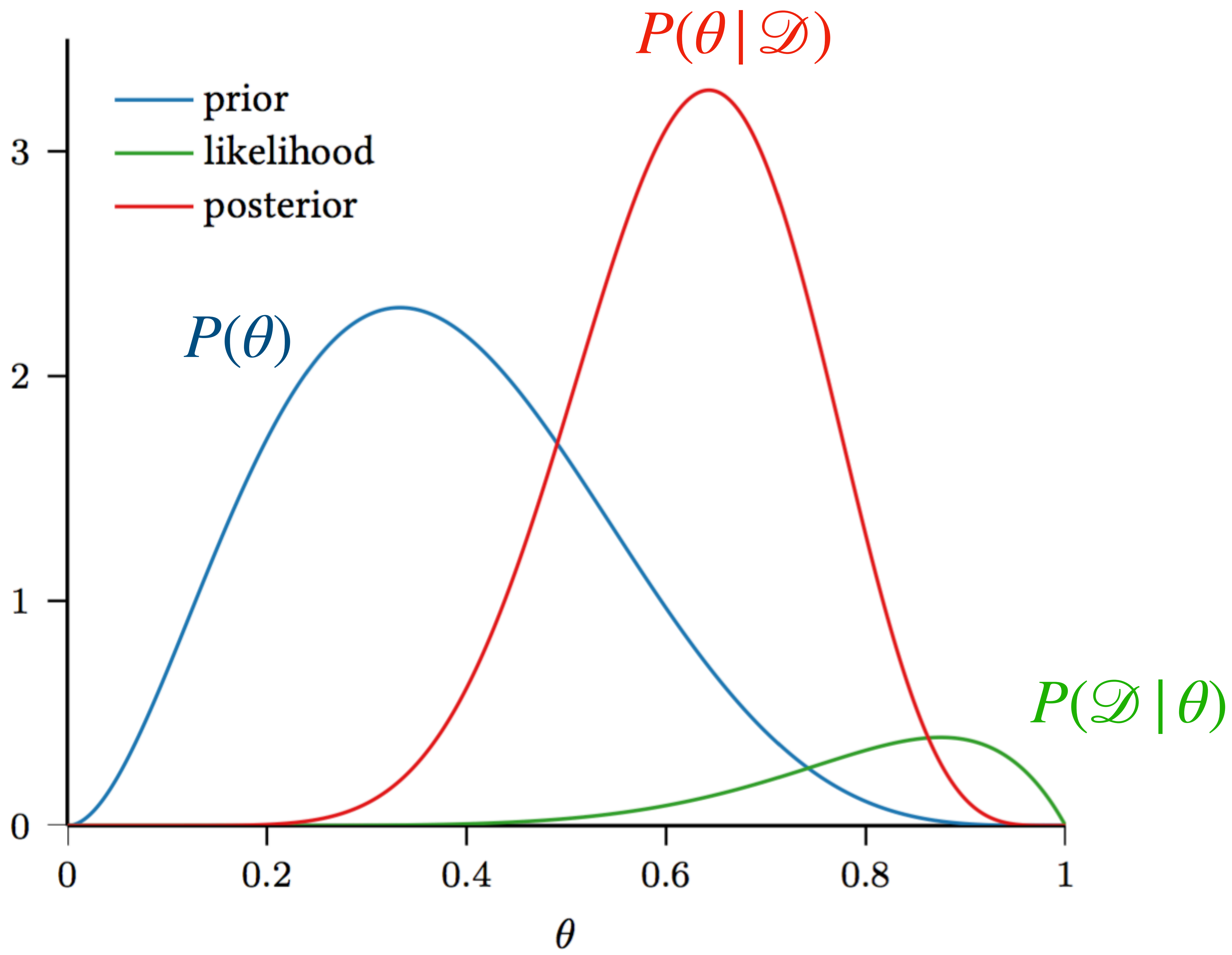
Some considerations on prior distributions

1. In coin flip example, when $n \to \infty, \hat{\theta}_{map} = \frac{n_1 + \alpha - 1}{n + \alpha + \beta - 2} \to \frac{n_1}{n}$(i.e.,$\hat{\theta}_{mle}$)

2. When n is small and our prior is accurate, MAP can work better than MLE

3. In general, not so easy to set up a good prior….

Summary



$P(\theta \mid \mathscr{D})$
prior
likelihood
posterior
3
2
1
0
$P(\theta)$
$P(\mathscr{D} \mid \theta)$
0
0.2
0.4
0.6
0.8
1
θ

Summary for today

1 MLE (frequentist perspective):

The ground truth $\theta^\star$ is unknown but fixed; we search for the parameter that makes the data as likely as possible

$$\arg\max_\theta P(\mathcal{D} \mid \theta)$$

2 MAP (Bayesian perspective):

The ground truth $\theta^\star$ treated as a random variable, i.e., $\theta^\star \sim P(\theta)$; we search for the parameter that maximizes the posterior

$$\arg\max_\theta P(\theta \mid \mathcal{D}) = \arg\max_\theta P(\theta)P(\mathcal{D} \mid \theta)$$